IN THE CLAIMS

Please cancel claims 2 and 69. In addition, please amend claims 1, 4, 5, 8, 9, 10, and 18 as shown below. Marked versions of amended claims 1, 4, 5, 8, 9, 10, and 18 showing all changes are attached hereto in Exhibit B.

Amended Claims:

1. A computer-aided method for the provision, identification and description of molecules exhibiting a desired activity comprising;

a molecular modeling step in which molecular descriptors are determined computationally;

a step of building a combinatorial library of molecules using said molecular descriptors;

a step of selecting candidate molecules which potentially exhibit said desired activity;

a filtering step whereby candidate molecules are filtered using at least one static filter representing a plurality of said molecular descriptors;

a further filtering step whereby candidate molecules are filtered using at least one dynamic filter representing constraints of conformational variations which each candidate molecule must satisfy in order to exhibit said desired activity.

4. A computer-aided method according to Claim 1 further comprising the step of screening the candidate molecules on the basis of the degree of enrichment provided by each candidate molecule to molecular descriptors.

5. A computer-aided method according to Claim 1 further comprising the step of deriving one or more criteria associating descriptor values with activity, said criteria including at least one static criterion and at least one dynamic criterion wherein at least one of said criteria is based on a non-linear function of a descriptor value.

8. A computer-aided method according to Claim 1 further comprising the step of deriving one or more criteria associating descriptor values with activity, said criteria including at least one static criterion and at least one dynamic criterion wherein at least one of said dynamic criteria is based on the conformational spaces of a candidate molecule.

9. A computer-aided method according to Claim 5 or Claim 8 wherein at least one of said dynamic criteria is based on a shape descriptor derived from a 3D autocorrelation vector (3D-ACV) of the candidate molecule.

10. A computer-aided method according to Claim 5, Claim 8 or Claim 9 wherein the static criteria are based on physiochemical and topological descriptors at least some of which are chosen from the following descriptors: Molar Mass; Ellipsoidal Volume; Molecular Volume; Molar Refractivity; Lipophilia (LogP); Kappa 1; Kappa 2; Kappa 3; Kappa Alpha 1; Kappa Alpha 2; Kappa Alpha 3; Flexibility; Kier Chi V4; Randic Index; Balaban Index; Weiner Index; Sum of Condition E; Dipolar Moment; Number of C Atoms; Number of O Atoms; Number of N Atoms; Number of H Atoms; Total Number of Atoms; Number of Methyl Groups; Number of Ethyl